Oct. 11, 2021

Bio-integrated Materials Science (Online Lectures)

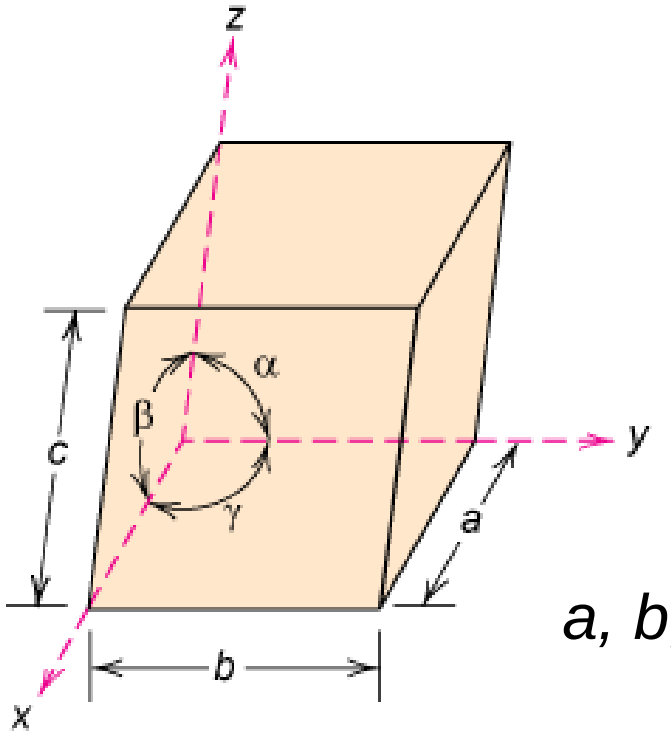
Crystal systems, Point coordinates, Crystallographic directions

Lecture 3

Prof. Jung Heon Lee

Crystal Systems

Unit cell: smallest [ ] volume which contains the complete lattice pattern of a crystal.



[ ] crystal systems

a, b, and *c* are the lattice constants

Fig. 3.20, *Callister & Rethwisch 4e.*

Table 3.6 Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

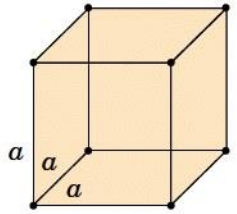
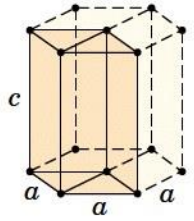
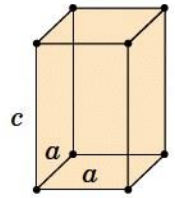
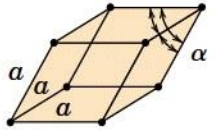
Crystal System	*Axial Relationships*	*Interaxial Angles*	*Unit Cell Geometry*
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	
Rhombohedral (Trigonal)	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	

Table 3.6 part 1

Table 3.6 Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

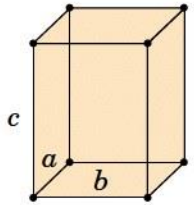
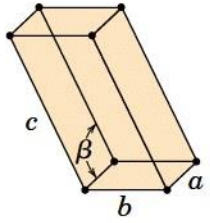
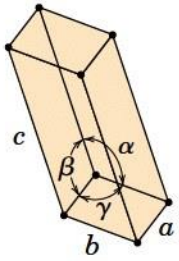
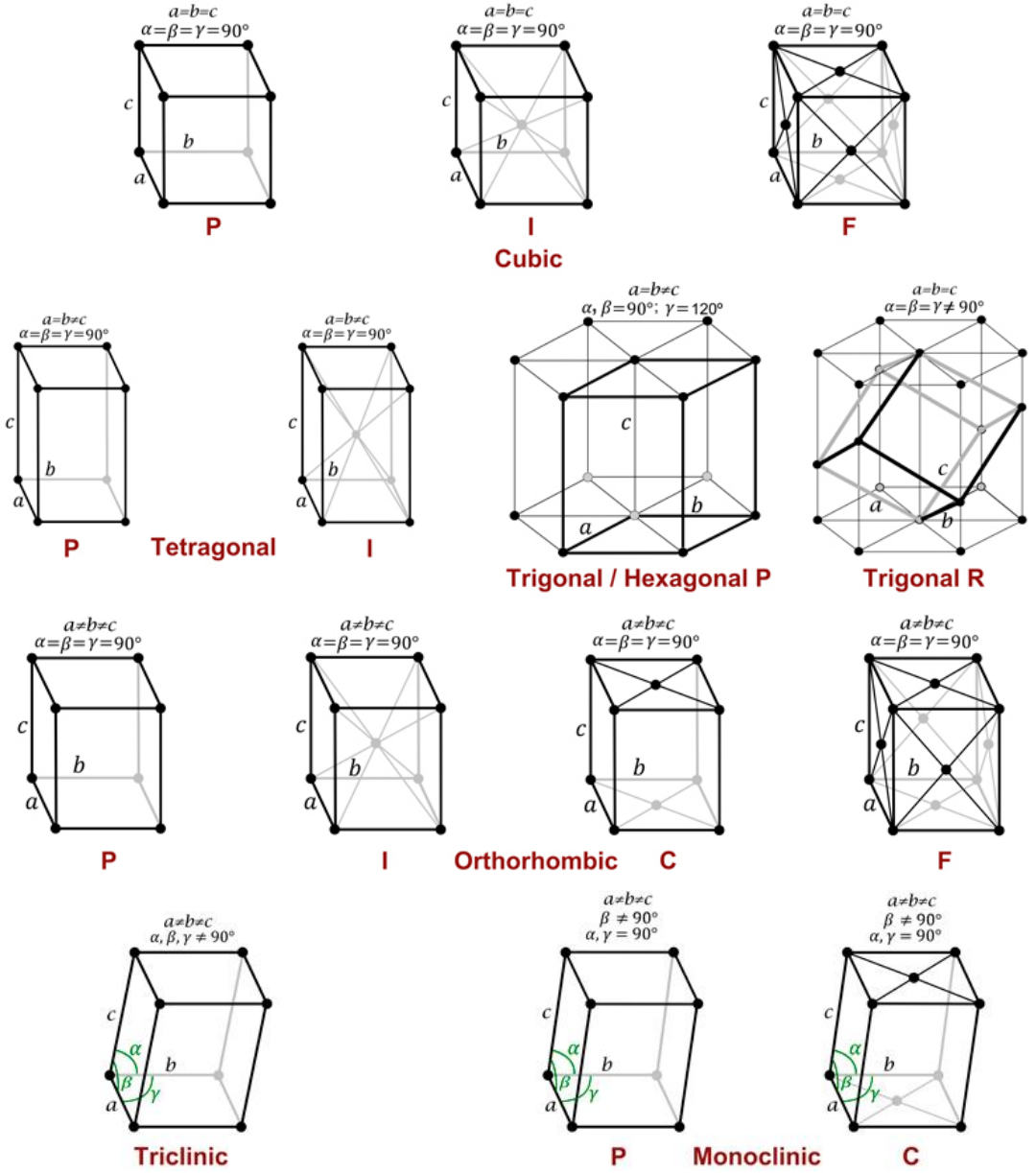
Crystal System	*Axial Relationships*	*Interaxial Angles*	*Unit Cell Geometry*
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	

Table 3.6 part 2

14 Bravais lattices



Symbols P C I F R refer to the different lattice types:

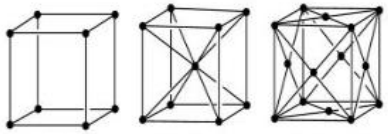
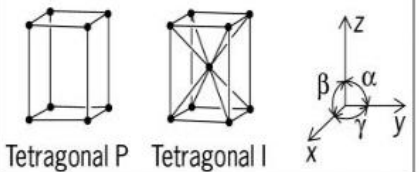
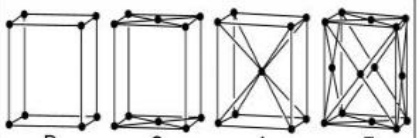
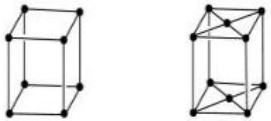
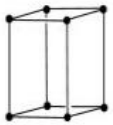
P = primitive (there is only one reticular point inside the cell (1 point in each of the 8 corners of the cell means 8/8=1 points in the cell)

C = centered in the faces perpendicular to the cell c axis (+ 1/8 of reticular point in each corner)

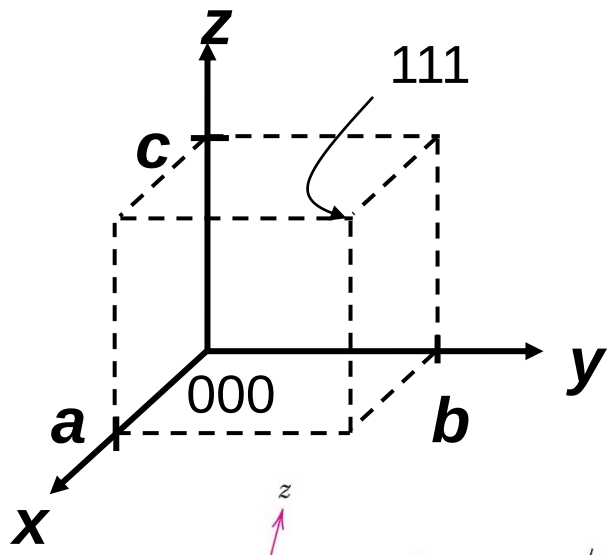
I = centered in the body of the cell (+ 1/8 of reticular point in each corner)

F = centered in all faces of the cell (+ 1/8 of reticular point in each corner)

R = primitive, identical cell axes and cell angles, or hexagonal two times body centered (+ 1/8 of reticular point in each corner)

Bravais lattice cells	Axes and interaxial angles	Examples
 Cubic P Cubic I Cubic F	Three axes at right angles; all equal: $a = b = c$; $\alpha = \beta = \gamma = 90°$	Copper (Cu), silver (Ag), sodium chloride (NaCl)
 Tetragonal P Tetragonal I	Three axes at right angles; two equal: $a = b \neq c$; $\alpha = \beta = \gamma = 90°$	White tin (Sn), rutile (TiO_2), β-spodumene ($LiAlSi_2O_6$)
 P C I F Orthorhombic	Three axes at right angles; all unequal: $a \neq b \neq c$; $\alpha = \beta = \gamma = 90°$	Gallium (Ga), perovskite ($CaTiO_3$)
 Monoclinic P Monoclinic C	Three axes, one pair not at right angles, of any lengths: $a \neq b \neq c$; $\alpha = \gamma = 90° \neq \beta$	Gypsum ($CaSO_4 \cdot 2H_2O$)
 Triclinic P	Three axes not at right angles, of any lengths: $a \neq b \neq c$; $\alpha \neq \beta \neq \gamma \neq 90°$	Potassium chromate (K_2CrO_7)
 Trigonal R (rhombohedral)	Rhombohedral: three axes equally inclined, not at right angles; all equal: $a = b = c$; $\alpha = \beta = \gamma \neq 90°$	Calcite ($CaCO_3$), arsenic (As), bismuth (Bi)
 Trigonal and hexagonal C (or P)	Hexagonal: three equal axes coplanar at 120°, fourth axis at right angles to these: $a_1 = a_2 = a_3 \neq c$; $\alpha = \beta = 90°$, $\gamma = 120°$	Zinc (Zn), cadmium (Cd), quartz (SiO_2) [P]

Point Coordinates



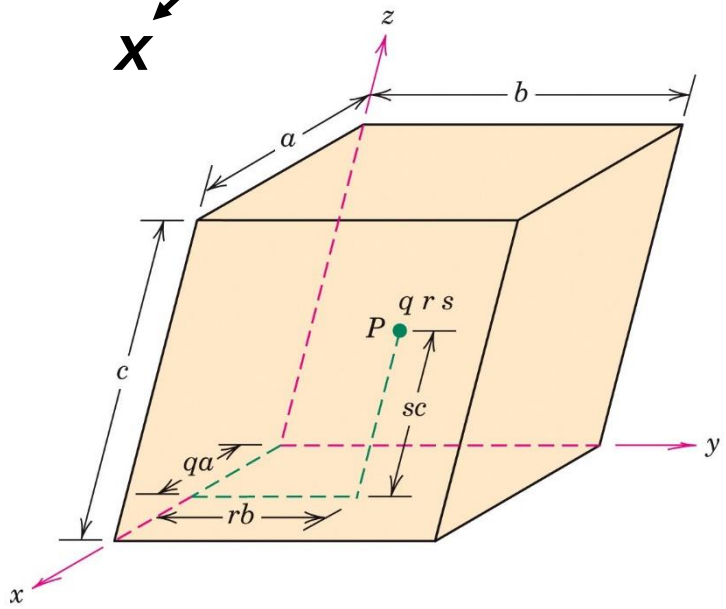


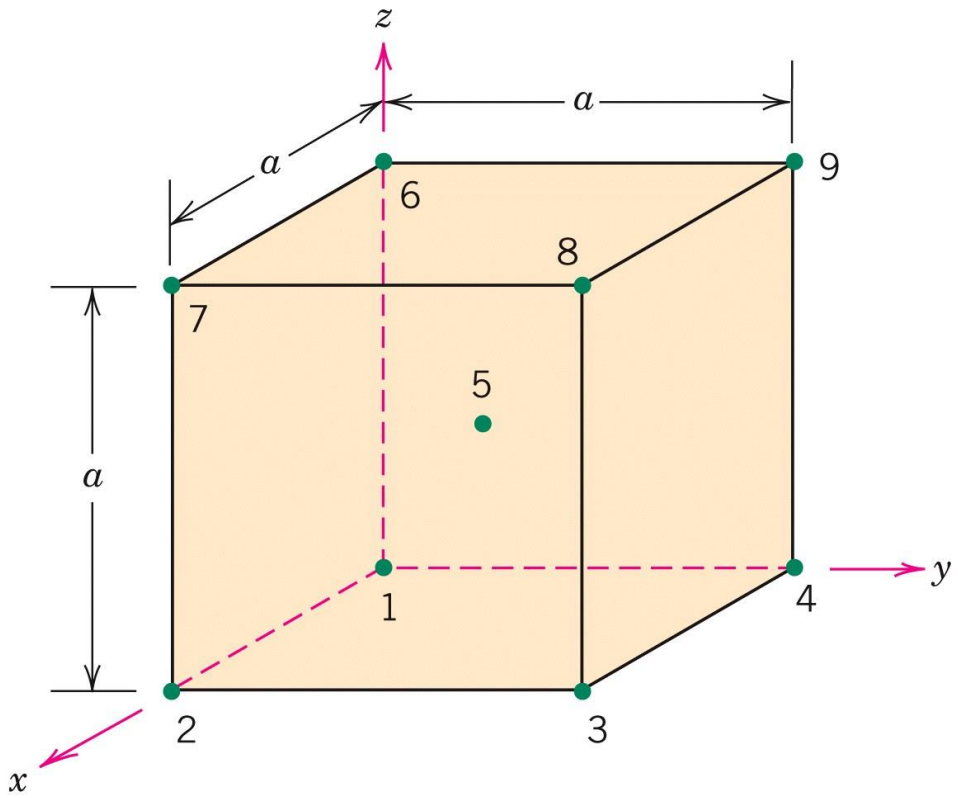
Figure 3.21

Point coordinates for unit cell center are

a/2, *b*/2, *c*/2

Point coordinates for unit cell corner are

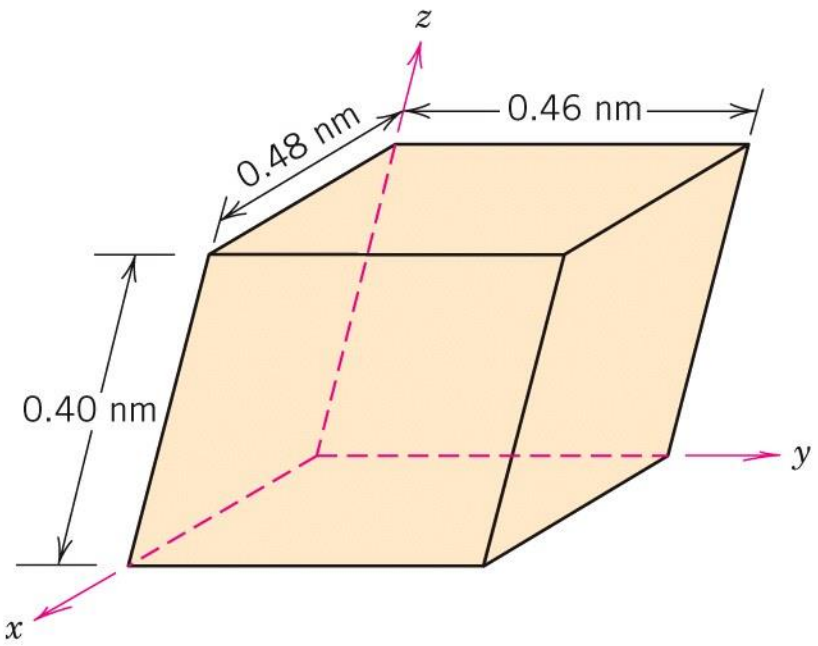
Translation: integer multiple of lattice constants → identical position in another unit cell

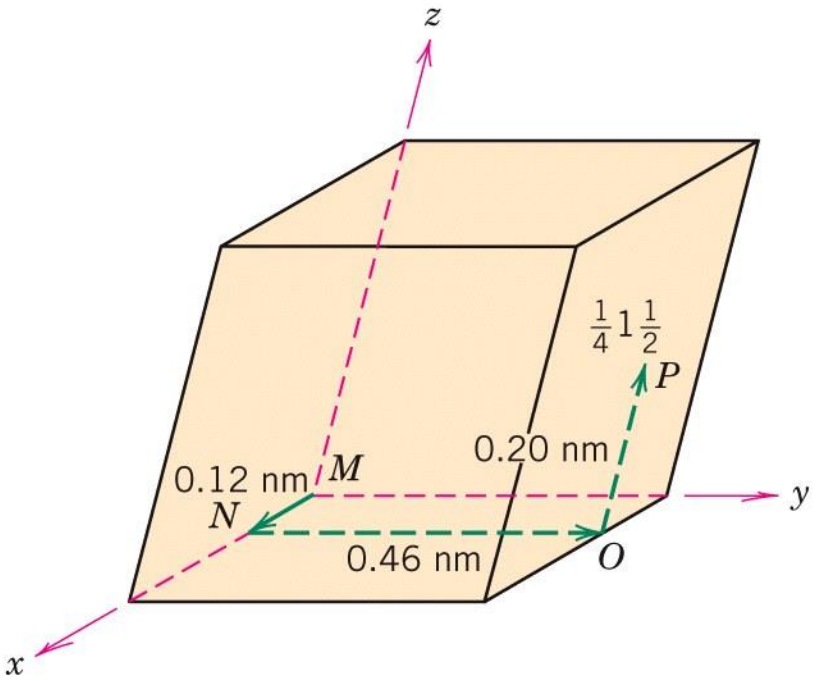


Unnumbered 3 p65b

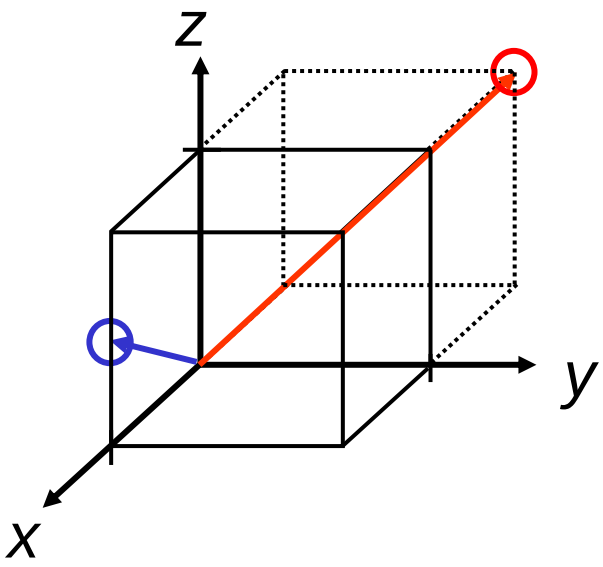
Point Number	Fractional Lengths			Point Coordinates
	x axis	y axis	z axis	
1	0	0	0	0 0 0
2	1	0	0	1 0 0
3	1	1	0	
4	0	1	0	
5	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	
6	0	0	1	
7	1	0	1	
8	1	1	1	
9	0	1	1	

Unnumbered 3 p66





Crystallographic Directions



Algorithm

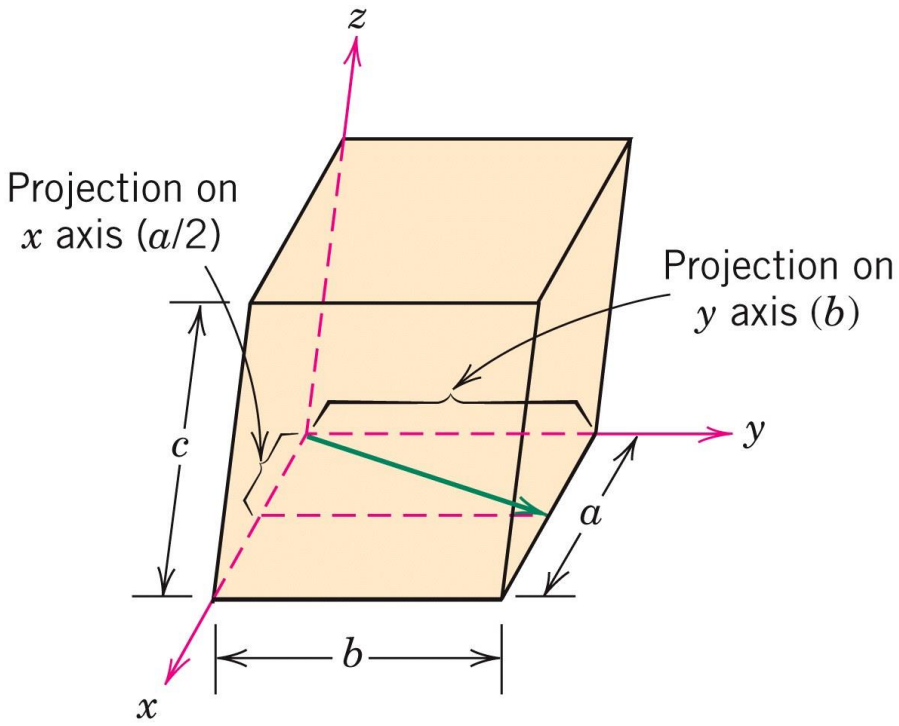
1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions *a*, *b*, and *c*
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas

[*uvw*]

ex: 1, 0, ½ => 2, 0, 1 => [ ]

[ ] => [ ] where overbar represents a negative index

families of directions <*uvw*>



Unnumbered 3 p67a

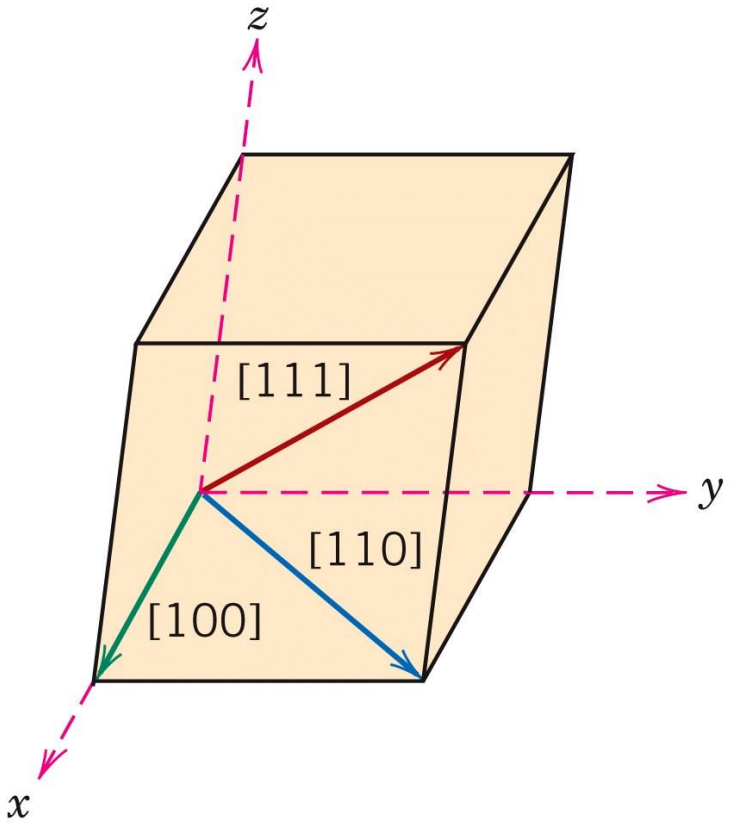
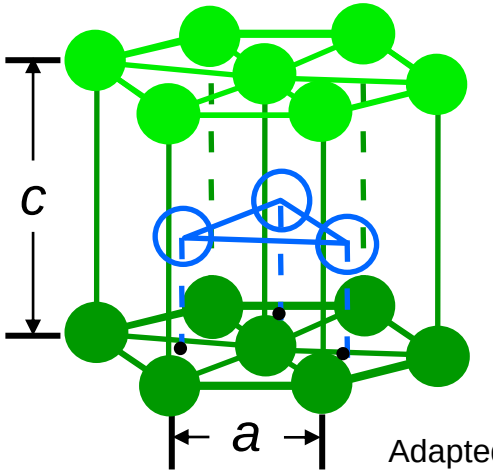


Figure 3.22

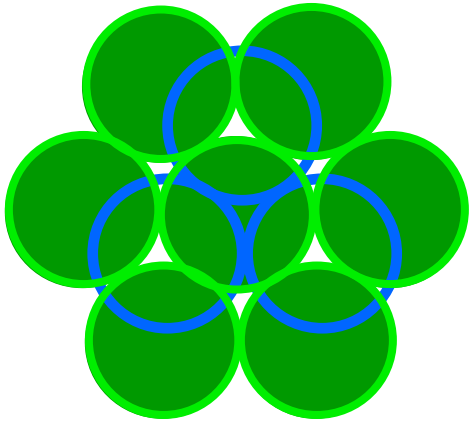
Hexagonal Close-Packed Structure (HCP)

- ABAB... Stacking Sequence
- 3D Projection



Adapted from Fig. 3.3(a), *Callister & Rethwisch 4e.*

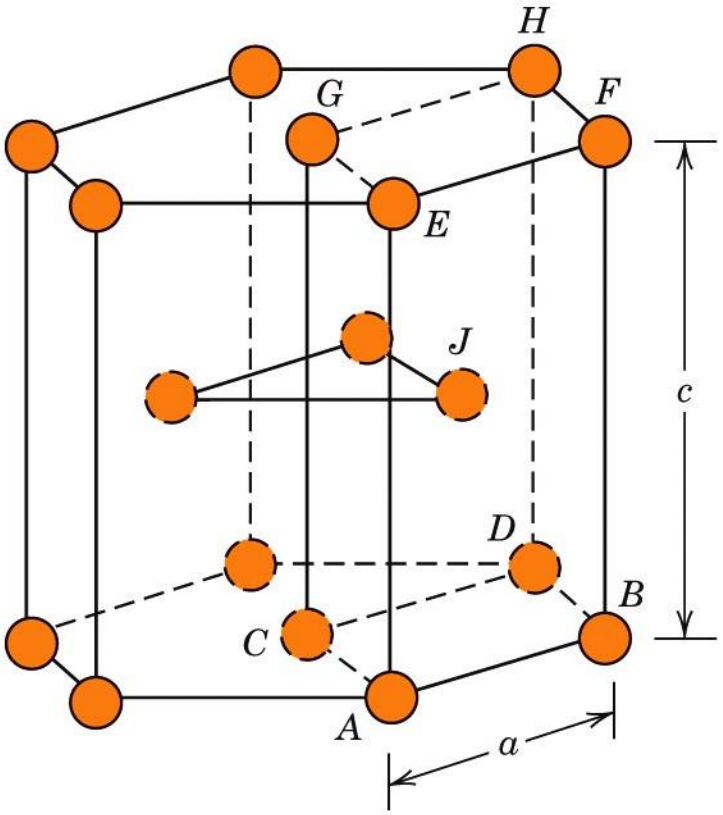
- 2D Projection



- Coordination # = 12
- APF = 0.74
- *c*/*a* = 1.633

6 atoms/unit cell

ex: Cd, Mg, Ti, Zn



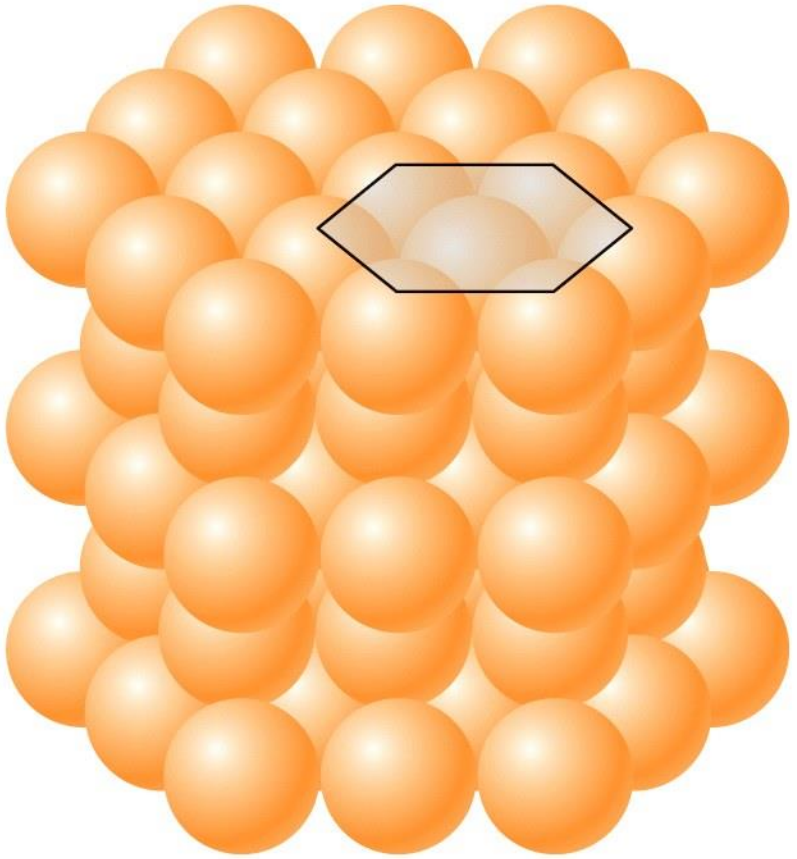


Figure 3.3

HCP Crystals

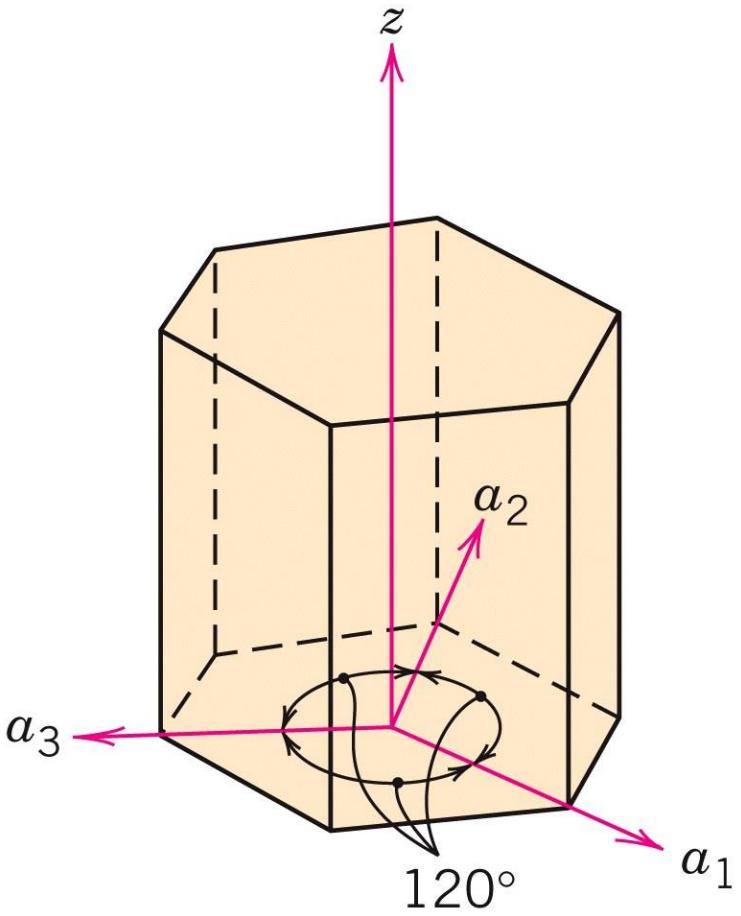


Figure 3.23

Coordinate axis system for a hexagonal unit cell (Miller–Bravais scheme)

- A four-axis (*Miller–Bravais)* coordinate system is used for hexagonal unit cell
- The three a_1, a_2, and a_3 axes are all contained within a single (basal) plane
- The z axis is perpendicular to this basal plane.
- Directional indices, which are obtained as described above, will be denoted by four indices, as [uvtw].

$$[u'v'w'] \longrightarrow [uvtw]$$

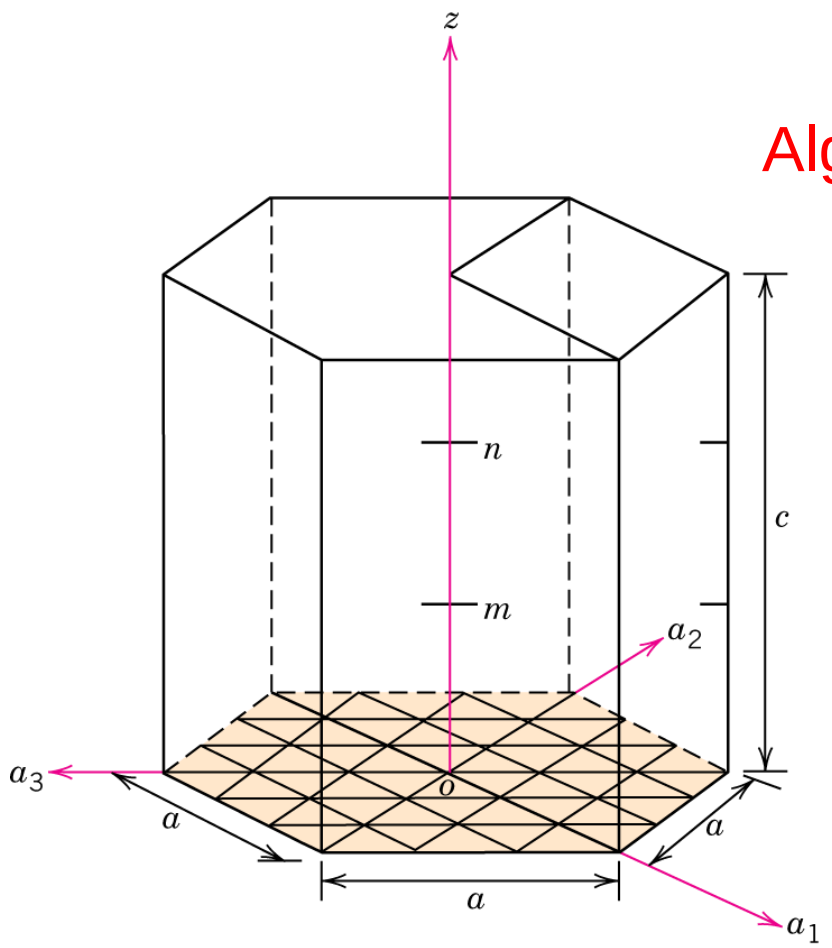
$$u = \frac{1}{3}(2u' - v')$$

$$v = \frac{1}{3}(2v' - u')$$

$$t = -(u + v)$$

$$w = w'$$

Drawing HCP Crystallographic Directions (i)



Adapted from Figure 3.25,
Callister & Rethwisch 4e.

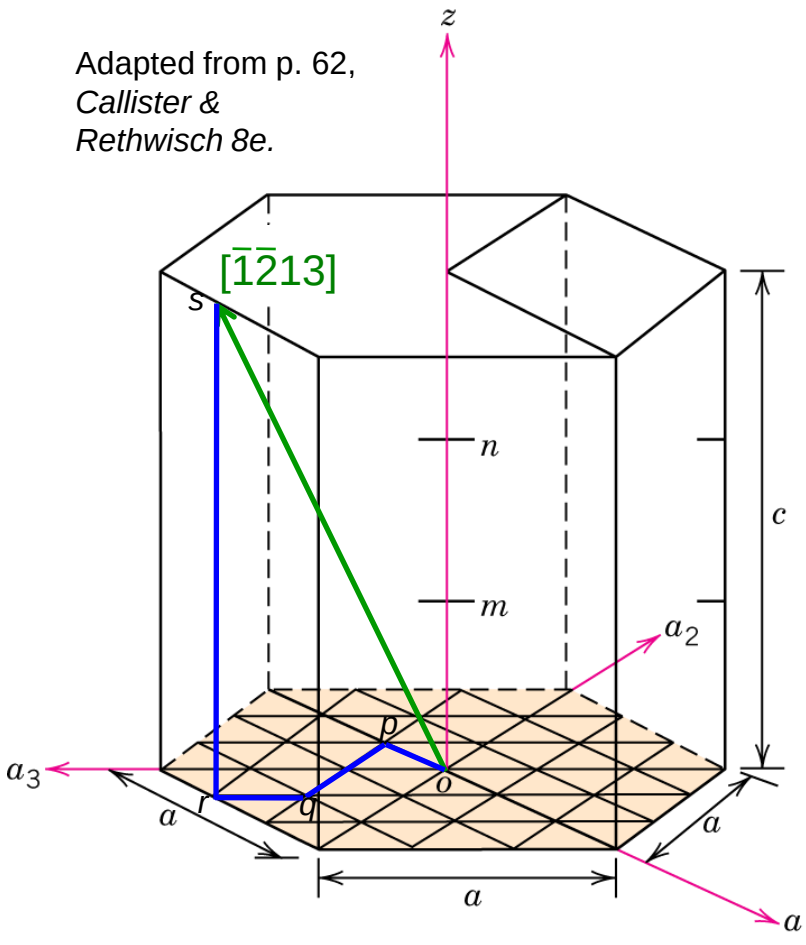
Algorithm (Miller-Bravais coordinates)

1. Remove brackets
2. Divide by largest integer so all values are ≤ 1
3. Multiply terms by appropriate unit cell dimension *a* (for a_1, a_2, and a_3 axes) or *c* (for *z*-axis) to produce projections
4. Construct vector by stepping off these projections

Determination of HCP Crystallographic Directions (ii)

- Draw the $[\bar{1}\,\bar{2}13]$ direction in a hexagonal unit cell.

Adapted from p. 62, *Callister & Rethwisch 8e.*



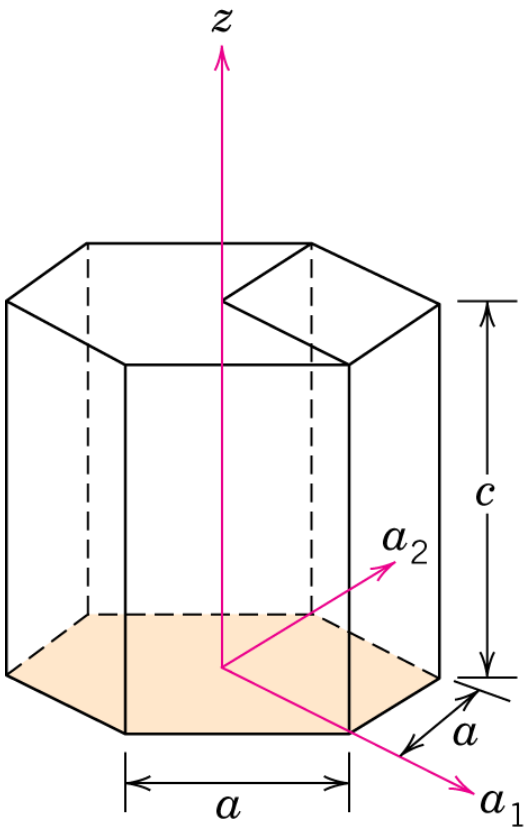
Algorithm

	a_1	a_2	a_3	z
1. Remove brackets				
2. Divide by 3				
3. Projections				

4. Construct Vector
   - start at point *o*
   - proceed $-a/3$ units along a_1 axis to point *p*
   - $-2a/3$ units parallel to a_2 axis to point *q*
   - $a/3$ units parallel to a_3 axis to point *r*
   - *c* units parallel to *z* axis to point *s*

$[\bar{1}\bar{2}13]$ direction represented by vector from point *o* to point *s*

Determination of HCP Crystallographic Directions (ii)



Adapted from p. 74, *Callister & Rethwisch 4e.*

Algorithm

1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of three-axis (a_1, a_2, and z) unit cell dimensions a and c
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas, for three-axis coordinates [$u'v'w'$]
5. Convert to four-axis Miller-Bravais lattice coordinates using equations below:

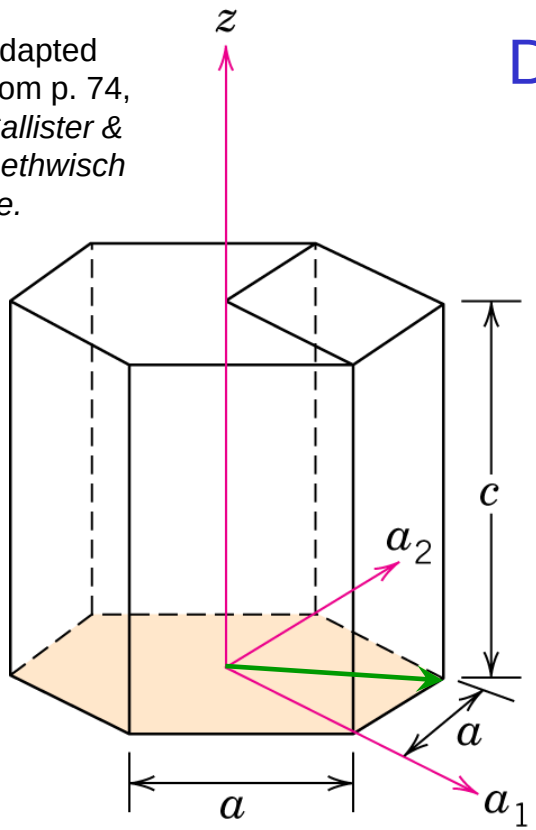
$$u = \frac{1}{3}(2u' - v') \qquad v = \frac{1}{3}(2v' - u')$$

$$t = -(u+v) \qquad w = w'$$

6. Adjust to smallest integer values and enclose in brackets [*uvtw*]

Determination of HCP Crystallographic Directions (ii)

Adapted from p. 74, *Callister & Rethwisch 4e.*



Determine indices for green vector

Example a_1 a_2 z

1. Reposition — not needed
2. Projections — a a $0c$
3. Reduction — 1 1 0
4. Brackets
5. Convert to 4-axis parameters

$u =$ $v =$

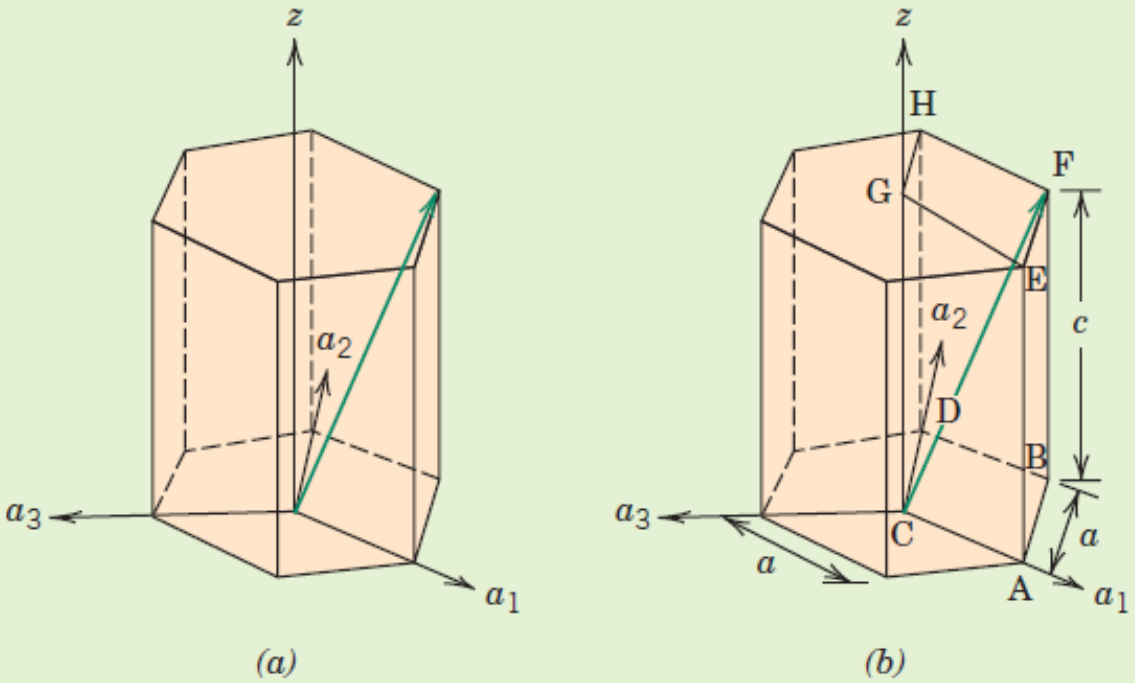
$t =$ $w =$

6. Reduction & Brackets

=> =>

Determination of Directional Indices for a Hexagonal Unit Cell

Determine the indices for the direction shown in the hexagonal unit cell of sketch (*a*) below.



Solution

In sketch (*b*), one of the three parallelepipeds comprising the hexagonal cell is delineated—its corners are labeled with letters A through H, with the origin of the a_1-a_2-a_3-z axes coordinate system located at the corner labeled C. We use this unit cell as a reference for specifying the directional indices. It now becomes necessary to determine projections of the direction vector on the a_1, a_2, and z axes. These respective projections are a (a_1 axis), a (a_2 axis) and c (z axis), which become 1, 1, and 1 in terms of the unit cell parameters. Thus,

Also, from Equations 3.6a, 3.6b, 3.6c, and 3.6d

$$u = \frac{1}{3}(2u' - v') =$$

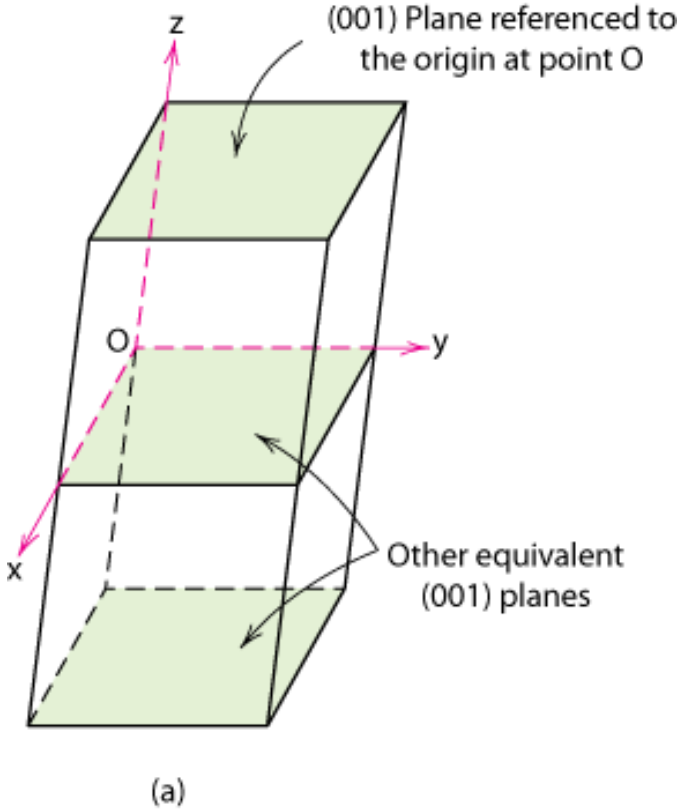
$$v = \frac{1}{3}(2v' - u') =$$

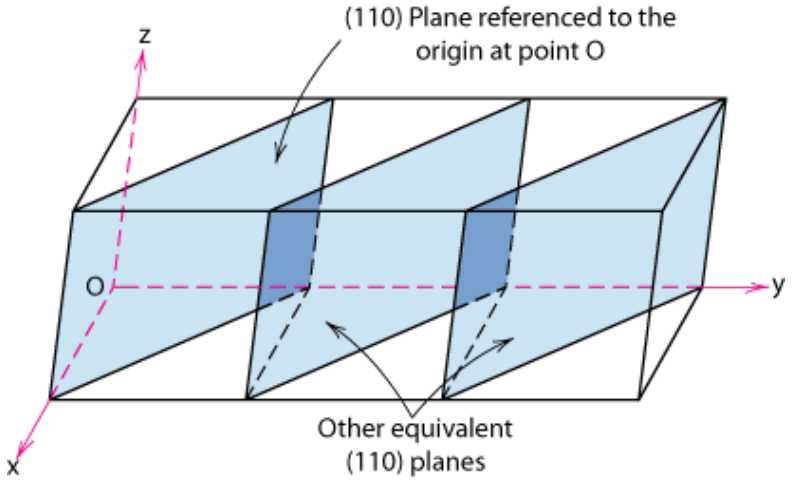
$$t = -(u + v) =$$

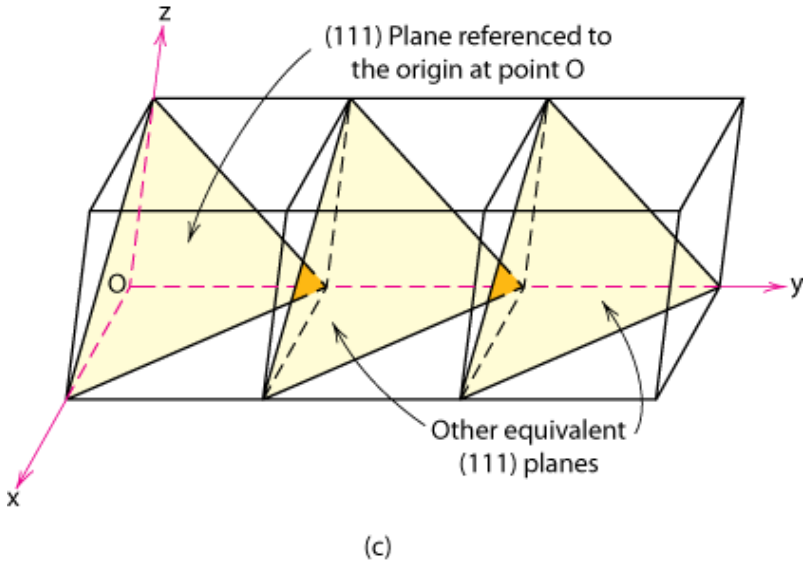
$$w = w' =$$

Multiplication of the above indices by 3 reduces them to the lowest set, which yields values for u, v, t, and w of 1, 1, −2 and 3, respectively. Hence, the direction shown in the figure is .

Crystallographic Planes







Adapted from Fig. 3.26,
Callister & Rethwisch 4e.

Crystallographic Planes

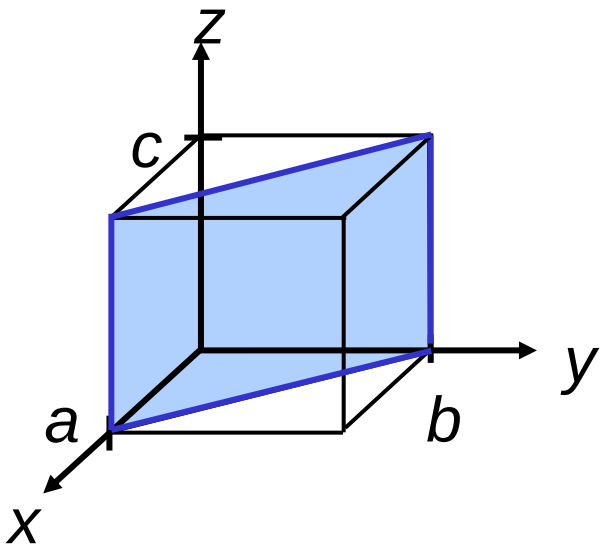
- Miller Indices: Reciprocals of the (three) axial intercepts for a plane, cleared of fractions & common multiples. All parallel planes have same Miller indices.

- Algorithm
  1. Read off intercepts of plane with axes in terms of *a*, *b*, *c*
  2. Take reciprocals of intercepts
  3. Reduce to smallest integer values
  4. Enclose in parentheses, no commas i.e., (*hkl*)

Crystallographic Planes

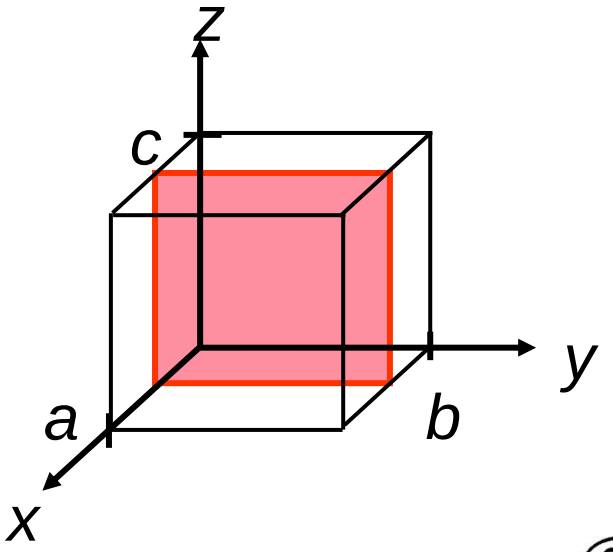
<u>example</u>

		a	b	c
1.	Intercepts			
2.	Reciprocals			
3.	Reduction			
4.	Miller Indices			



<u>example</u>

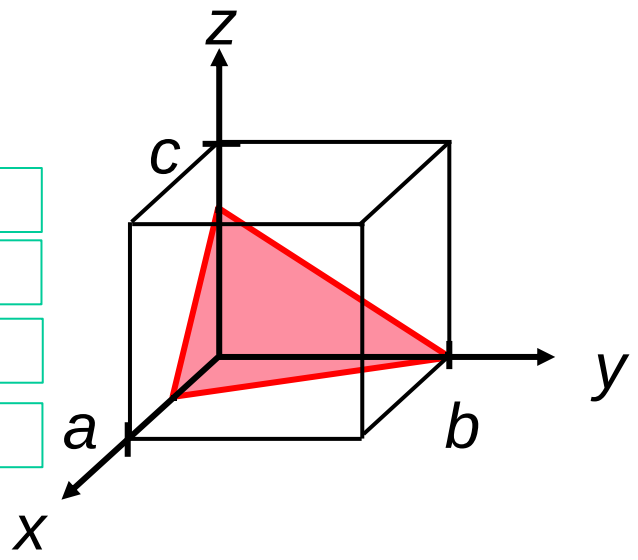
		a	b	c
1.	Intercepts			
2.	Reciprocals			
3.	Reduction			
4.	Miller Indices			



Crystallographic Planes

example

	a	b	c
1. Intercepts			
2. Reciprocals			
3. Reduction			
4. Miller Indices			



Family of Planes {*hkl*}

Ex: {100} = (100), (010), (001), $(\bar{1}00)$, $(0\bar{1}0)$, $(00\bar{1})$

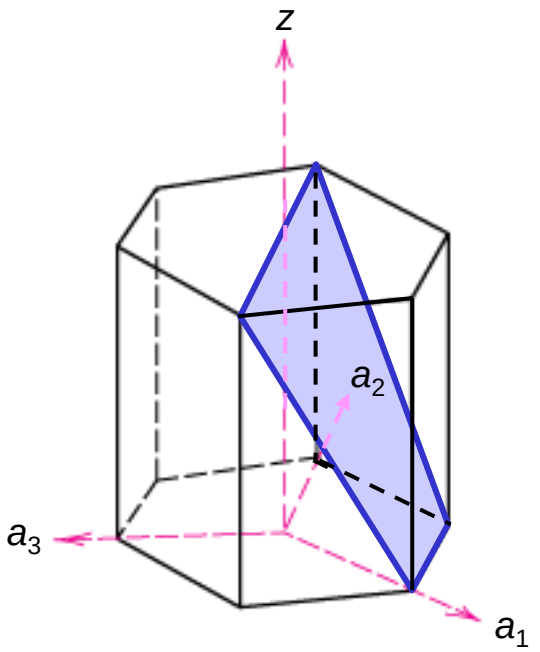
Crystallographic Planes (HCP)

- In hexagonal unit cells the same idea is used

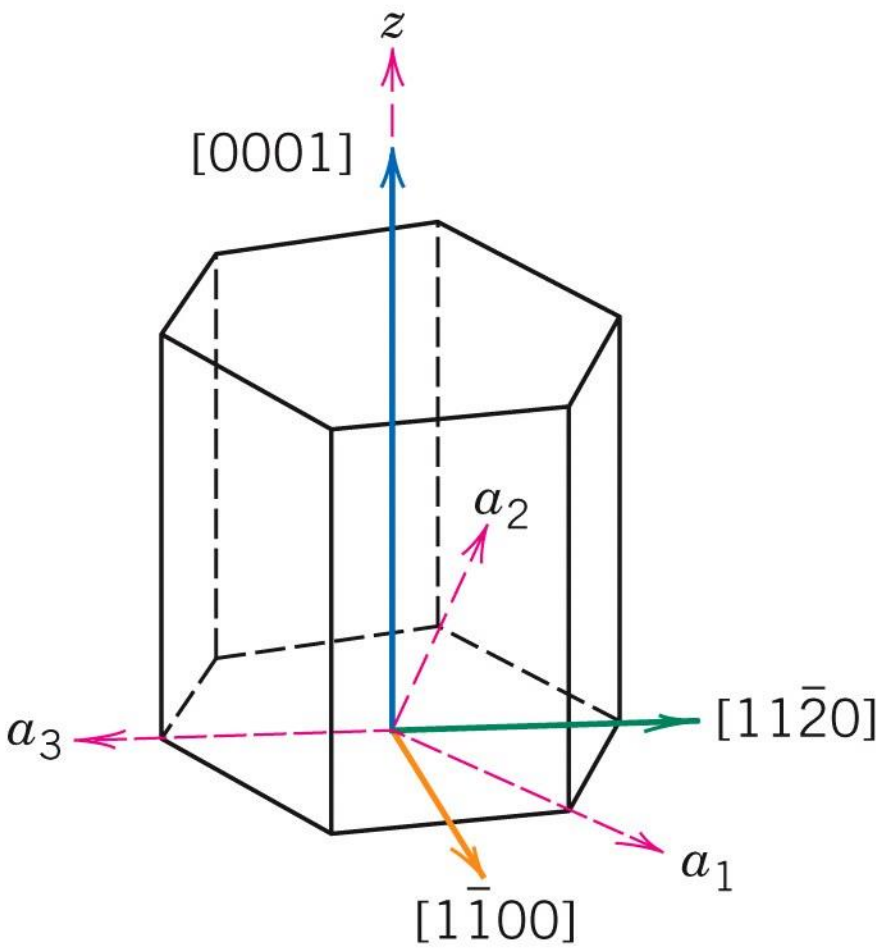
example

	a_1	a_2	a_3	c
1. Intercepts				
2. Reciprocals				
3. Reduction				

4. Miller-Bravais Indices



Adapted from Fig. 3.24(b), *Callister & Rethwisch 4e.*



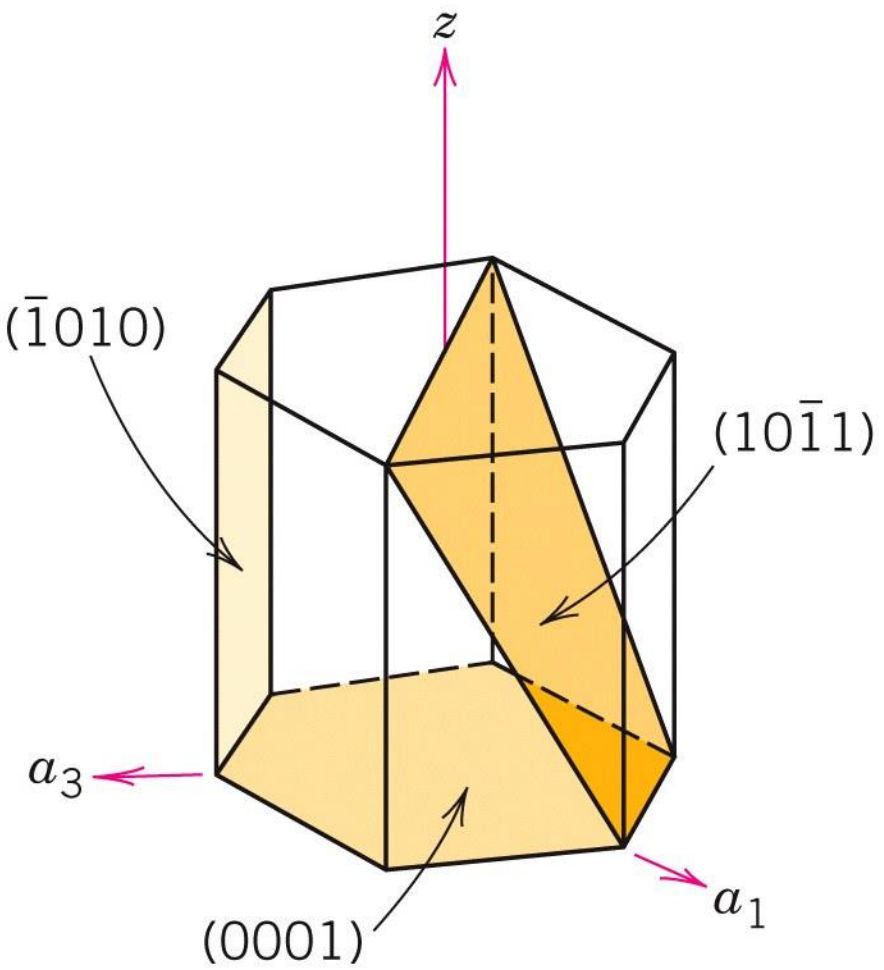


Figure 3.24

Single crystal

The
Royal Sceptre
- Cullinan I

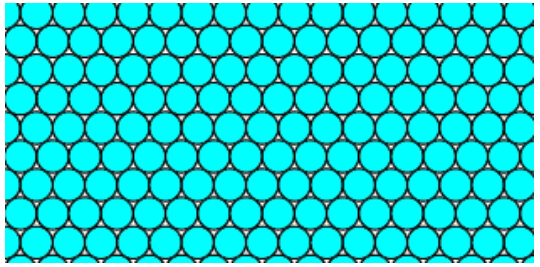
Imperial State
Crown of Great
Britain - Cullinan II

Single crystal
Si

Grains

- Crystalline: a single crystallite in a material (grain)

  FCC, BCC, HCP, …..



- Polycrystalline: multiple single crystallites coexisting in a material

- Grain boundaries: boundaries existing between different crystallites